

# Adiabatic transport in nanostructures

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A confined system of non-interacting electrons, subject to the combined effect of a time-dependent potential and different external chemical-potentials, is considered. The current flowing through such a system is obtained for arbitrary strengths of the modulating potential, using the adiabatic approximation in an iterative manner. A new formula is derived for the charge pumped through an un-biased system (all external chemical potentials are kept at the same value); It reproduces the Brouwer formula for a two-terminal nanostructure. The formalism presented yields the effect of the chemical potential bias on the pumped charge on one hand, and the modification of the Landauer formula (which gives the current in response to a constant chemical-potential difference) brought about by the modulating potential on the other. Corrections to the adiabatic approximation are derived and discussed.

73.23.-b, 73.63.Rt, 73.50.Rb, 73.40.Ei

## I. INTRODUCTION AND SUMMARY

The flow of a dc current in response to a slowly-varying time-dependent potential operating on an *un-biased* system is termed “adiabatic charge pumping”.<sup>1</sup> This phenomenon, first considered in Ref. 2, has attracted recently much theoretical<sup>3–14</sup> and experimental<sup>15–17</sup> interest. In general, “adiabatic pumping” occurs when the charge transferred across a boundary during a single period of a certain modulating potential is independent of the modulation frequency. This process is adiabatic in the sense that the periodic potential varies very slowly in time, such that its frequency  $\omega$  is smaller than any characteristic energy scale of the electrons.

Eighteen years ago, Thouless<sup>18</sup> has shown, using the adiabatic approximation, that the ground state of an infinite one-dimensional (1D) system of non-interacting electrons subject to a slowly moving periodic potential can support a dc current. Later theoretical investigations of quantum pumping in confined nanostructures have employed the result derived by Brouwer,<sup>3</sup> which gives the pumped charge in terms of the time-dependent scattering matrix related to the modulating potential. The derivation presented by Brouwer is based on the analysis of Ref. 19, which, in turn, utilizes an expansion in the amplitude of the modulating potential in the context of time-dependent scattering theory. Nevertheless, it is generally accepted that the formalism of Büttiker *et al.*<sup>19</sup> and the resulting Brouwer formula are valid<sup>20</sup> even for large amplitudes, as long as the adiabatic approximation holds.

This paper is devoted, among other issues, to the exploration of this point. We consider a spatially-confined system of non-interacting electrons, connected by leads (denoted by  $\alpha$ ) to electronic reservoirs which are kept at various chemical potentials,  $\mu_\alpha$ . The system is also

subject to a slowly-varying periodic potential. We derive an expression for the instantaneous current flowing in this system, allowing for arbitrary strengths of the modulating potential, using time-dependent scattering states. The formalism is based on an iterative solution of those states, in the adiabatic approximation, in which the temporal derivative of the scattering potential (and the scattering states) is the small parameter. The formal derivation is summarized in Sec. II, where we obtain the instantaneous current in the lowest-order adiabatic approximation. This current is averaged over a single period of the modulating potential. In this way we obtain the effect of the chemical potential bias on the pumped charge on one hand, and the modification of the Landauer formula caused by the modulating potential on the other. We find a new expression for the charge pumped through an un-biased system [see Eq. (1) below], which is particularly useful in cases where the modulating potential operates on the entire nanostructure,<sup>21</sup> and is spatially-dependent. The Appendix includes the derivation of the next order correction to the current.

We investigate the lowest-order expression for the current in Sec. III, confining ourselves for simplicity to a system connected to two reservoirs. Our results there can be summarized as follow. In a two-terminal structure, the current averaged over a single period,  $\tau$ , consists of two parts. The first, denoted by  $I_{\text{pump}}$ , flows even when the system is un-biased, (but is modified by the presence of the chemical potential difference). To the lowest order in the adiabatic approximation, that current reads

$$I_{\text{pump}} = \frac{e}{4\pi} \oint \frac{dt}{\tau} \int dE \left( -\frac{\partial}{\partial E} (f_\ell(E) + f_r(E)) \right) \times \sum_m \left[ \langle rm | \dot{V} | rm \rangle - \langle \ell m | \dot{V} | \ell m \rangle \right], \quad (1)$$

where  $\ell$  and  $r$  denote the left and the right leads, respectively, and  $f_{\ell,r}(E) \equiv (e^{(E-\mu_{\ell,r})/k_B T} + 1)^{-1}$  are the Fermi distributions in the reservoirs connected to the left and right leads. In Eq. (1),  $|\beta m\rangle \equiv \chi_{\beta m}^t$  is the instantaneous scattering state at time  $t$ , excited by an incoming wave in channel  $m$  of lead  $\beta$ , and  $\dot{V}$  is the temporal derivative of the time-dependent scattering potential. Interestingly enough, the matrix element appearing in Eq. (1) can be written in terms of the instantaneous scattering matrix, reproducing the Brouwer formula,<sup>3</sup> and vindicating its use for arbitrary amplitudes. The second part of the current, denoted by  $I_{\text{bias}}$ , flows only when the system is biased, i.e.,  $\mu_\ell \neq \mu_r$ . When this current is integrated over a single period,  $\tau$ , of the modulating potential, one obtains the Landauer formula, modified by the modulated potential in two ways: (i) The transmission coefficient is the instantaneous one,  $T^t$ , averaged over a single period of the time-dependent potential; (ii) There appears a correction to the Landauer expression, which is related to the temporal derivative of the modulating potential and the ensuing instantaneous scattering matrix. In the simplest case in which the two leads are single-channel ones,  $I_{\text{bias}}$  takes a particularly simple form,

$$I_{\text{bias}} = \frac{e}{\tau\pi} \oint dt \int dE \times \left[ T^t + \frac{1}{2} T^t \frac{d\psi^t}{dt} \frac{\partial}{\partial E} \right] (f_\ell(E) - f_r(E)), \quad (2)$$

in which  $\psi^t$  is the instantaneous Friedel phase (i.e., the transmission phase) of the nanostructure. The first term in Eq. (2) yields the Landauer formula for the present case. The second term there is a correction, which is discussed in Sec. III, using a simple example.

## II. TIME-DEPENDENT SCATTERING THEORY IN THE ADIABATIC APPROXIMATION

In the first part of this section we solve for the time-dependent scattering states iteratively, using the adiabatic approximation. We then use those scattering states in the second part, to obtain the current. The formalism presented below borrows from the derivations in Refs. 22 and 23, extended to include the effect of a time-dependent scattering potential.

### A. Time-dependent scattering states

We consider a ballistic nanostructure of arbitrary geometry, which consists of a nanostructure connected to several electronic reservoirs. This system is described by the Hamiltonian

$$\mathcal{H}(\mathbf{r}, t) = \mathcal{H}_0(\mathbf{r}) + V(\mathbf{r}, t), \quad (3)$$

where the scattering potential  $V(\mathbf{r}, t)$  is assumed to be confined in space, so that asymptotic behaviors of the

scattering solutions can be defined un-ambiguously. This confined region is attached to leads, numbered by the index  $\alpha$ , and each lead is connected to a reservoir having the chemical potential  $\mu_\alpha$ . The Hamiltonian  $\mathcal{H}_0$  consists of the kinetic energy. We use the adiabatic approximation, requiring that the characteristic inverse time-constant,  $1/\tau$ , which describes the time dependence of  $V$ , is smaller than any characteristic energy scale of the electrons. For a simple oscillatory potential,  $\tau = 2\pi/\omega$ .

As in the usual scattering treatment, we denote the incoming wave with energy  $E$  in lead  $\alpha$  by  $w_{\alpha n}^-$ , where  $n$  is the transverse mode number. This wave is a solution of the free Hamiltonian,

$$(\mathcal{H}_0(\mathbf{r}) - E)w_{\alpha n}^-(\mathbf{r}) = 0, \quad (4)$$

and is normalized such that it carries a unit flux. The scattering solution of the full Hamiltonian, excited by this incoming wave, can be written in the form

$$\begin{aligned} \Psi_{\alpha n}(\mathbf{r}, t) &= e^{-iEt} \chi_{\alpha n}(\mathbf{r}, t), \\ \chi_{\alpha n}(\mathbf{r}, t) &= w_{\alpha n}^-(\mathbf{r}) + \tilde{\chi}_{\alpha n}(\mathbf{r}, t). \end{aligned} \quad (5)$$

The time dependence of the scattered wave function,  $\tilde{\chi}_{\alpha n}(\mathbf{r}, t)$ , is expected to have the same characteristic time scale as  $V$ . For example, when the modulating potential is oscillating in time,  $\tilde{\chi}$  contains all harmonics of the frequency  $\omega$ .

The scattering solution  $\Psi_{\alpha n}$  should satisfy the time-dependent Schrödinger equation,

$$i \frac{\partial \Psi_{\alpha n}(\mathbf{r}, t)}{\partial t} = \mathcal{H}(\mathbf{r}, t) \Psi_{\alpha n}(\mathbf{r}, t). \quad (6)$$

Inserting (5) into (6), using Eq. (4), we find

$$\left( G^t(E) \right)^{-1} \tilde{\chi}_{\alpha n}(\mathbf{r}, t) = V(\mathbf{r}, t) w_{\alpha n}^-(\mathbf{r}) - i \frac{\partial \tilde{\chi}_{\alpha n}(\mathbf{r}, t)}{\partial t}, \quad (7)$$

where  $G^t$  is the instantaneous Green function of the full Hamiltonian, such that

$$(E - \mathcal{H}(\mathbf{r}, t)) G^t(E; \mathbf{r}, \mathbf{r}') = \delta(\mathbf{r}' - \mathbf{r}). \quad (8)$$

We now solve Eq. (7), using the adiabatic approximation: the temporal derivative appearing on the right-hand-side of that equation is regarded as a small correction (of order  $1/\tau$ ), and the equation is solved iteratively. The zeroth-order is just the instantaneous scattering solution, which we denote by  $\chi_{\alpha n}^t$ ,

$$\chi_{\alpha n}^t(\mathbf{r}) = w_{\alpha n}^-(\mathbf{r}) + \int d\mathbf{r}' G^t(E; \mathbf{r}, \mathbf{r}') V(\mathbf{r}', t) w_{\alpha n}^-(\mathbf{r}'). \quad (9)$$

The instantaneous scattering state  $\chi_{\alpha n}^t$  is the solution of the instantaneous Schrödinger equation, with energy  $E$ ,

$$(E - \mathcal{H}(\mathbf{r}, t)) \chi_{\alpha n}^t(\mathbf{r}) = 0. \quad (10)$$

Turning back to Eq. (7), one finds that to first order in the time-derivative the scattering solution reads

$$\chi_{\alpha n}(\mathbf{r}, t) = \chi_{\alpha n}^t(\mathbf{r}) - i \int d\mathbf{r}' G^t(E; \mathbf{r}, \mathbf{r}') \dot{\chi}_{\alpha n}^t(\mathbf{r}'), \quad (11)$$

in which  $\dot{\chi}_{\alpha n}^t$  is the time-derivative of the instantaneous scattering state. Hence, to first order in the adiabatic approximation the time-dependent scattering states are given entirely in terms of the *instantaneous* solutions (namely,  $\chi_{\alpha n}^t$  and  $G^t(E; \mathbf{r}, \mathbf{r}')$ ) of the problem at hand. One notes that the adiabatic solution (11) of the scattering state is analogous to Thouless<sup>18</sup> solution for the ground-state wave function in his model. In the Appendix, we discuss the corrections to the lowest order adiabatic approximation.

## B. The current

Here we outline the derivation of the current in the scattering states formalism, as developed, e.g., in Refs. 22, 23, and 24. One writes the field operator of the electron,  $\hat{\Psi}(\mathbf{r}, t)$ , in terms of the scattering states as

$$\hat{\Psi}(\mathbf{r}, t) = \int \frac{dE}{2\pi} \sum_{\alpha} \hat{a}_{\alpha n}(E) e^{-iEt} \chi_{\alpha n}(\mathbf{r}, t), \quad (12)$$

in which  $\hat{a}_{\alpha n}$  destroys an electron incoming in channel  $n$  of lead  $\alpha$ . The thermal average of the latter operators is given by the Fermi distributions of the various reservoirs, such that

$$\langle \hat{a}_{\alpha n}^\dagger(E) \hat{a}_{\alpha' n'}(E') \rangle = 2\pi \delta(E - E') \delta_{\alpha n, \alpha' n'} f_{\alpha}(E), \quad (13)$$

where  $f_{\alpha}(E)$  is the Fermi distribution in the reservoir connected to the  $\alpha$  lead. With these definitions, the thermal average of the current density operator becomes

$$\langle \mathbf{j}(\mathbf{r}, t) \rangle = \frac{e}{m} \Im \int \frac{dE}{2\pi} \sum_{\alpha} f_{\alpha}(E) \chi_{\alpha n}^*(\mathbf{r}, t) \frac{\partial \chi_{\alpha n}(\mathbf{r}, t)}{\partial \mathbf{r}}, \quad (14)$$

where  $e$  stands for the negative electron charge.

It is convenient to evaluate this quantity when  $\mathbf{r}$  approaches  $\infty$  in lead  $\beta$  (which will be denoted by  $\mathbf{r} \rightarrow \infty\beta$ ), and then to integrate the current density over the cross-section of that lead (noting that the incoming and outgoing waves are normalized to carry a unit flux). In so doing, we may take advantage of the asymptotic properties of the instantaneous quantities  $\chi_{\alpha n}^t$  and  $G^t(E)$ , as documented in Refs. 22 and 24,

$$\begin{aligned} G^t(E; \mathbf{r}, \mathbf{r}')|_{\mathbf{r} \rightarrow \infty\beta} &= -i \sum_m w_{\beta m}^+(\mathbf{r}) \chi_{\beta m}^t(\mathbf{r}'), \\ \chi_{\alpha n}^t(\mathbf{r})|_{\mathbf{r} \rightarrow \infty\beta} &= \delta_{\alpha\beta} w_{\alpha n}^-(\mathbf{r}) + \sum_m w_{\beta m}^+(\mathbf{r}) S_{\beta m, \alpha n}^t. \end{aligned} \quad (15)$$

Here,  $w_{\beta m}^+$  is the outgoing wave in channel  $m$  of lead  $\beta$  and  $S_{\beta m, \alpha n}^t$  is the matrix element of the instantaneous

scattering matrix. As a result, the current flowing into lead  $\beta$  is given by

$$\begin{aligned} I_{\beta}(t) &= e \int \frac{dE}{2\pi} \sum_{\alpha n} f_{\alpha}(E) \\ &\times \left( \delta_{\alpha\beta} - \sum_m \left[ |S_{\beta m, \alpha n}^t|^2 - 2\Re \left( S_{\beta m, \alpha n}^t U_{\beta m, \alpha n}^* \right) \right] \right), \end{aligned} \quad (16)$$

with

$$U_{\beta m, \alpha n} = \int d\mathbf{r} \chi_{\beta m}^t(\mathbf{r}) \dot{\chi}_{\alpha n}^t(\mathbf{r}). \quad (17)$$

The result (16) for the time-dependent current entering into lead  $\beta$  of the nanostructure holds for a general biased system, whose various terminals have different chemical potentials (as long as the time-dependence of the periodic potential is slow enough). It is therefore interesting to consider charge conservation, using that result. Indeed, summing (16) over all leads, we obtain

$$\sum_{\beta} I_{\beta}(t) = e \int \frac{dE}{2\pi} \sum_{\alpha n} f_{\alpha}(E) \frac{d}{dt} \int d\mathbf{r} |\chi_{\alpha n}^t(\mathbf{r})|^2, \quad (18)$$

which shows that when the total current entering the system,  $\sum_{\beta} I_{\beta}(t)$ , is integrated over a single period of the modulating potential, the result is zero, i.e., the charge per period is conserved. In deriving the result (18) we have employed (i) the unitarity of the instantaneous scattering matrix,  $\sum_{\beta m} S_{\beta m, \alpha n}^{t*} S_{\beta m, \alpha' n'}^t = \delta_{\alpha n, \alpha' n'}$ ; and (ii) the following property of the scattering matrix<sup>22,24</sup>

$$\sum_{\beta m} S_{\beta m, \alpha n}^{t*} \chi_{\beta m}^t(\mathbf{r}) = \chi_{\alpha n}^{t*}(\mathbf{r}). \quad (19)$$

Equation (16) can be considered as a generalization of the Landauer formula, extended to include the effect of a time-dependent potential, in the adiabatic approximation. The new ingredient is the quantity  $U_{\alpha n, \beta m}$ , Eq. (17). This quantity can be expressed in terms of the temporal derivative of the scattering potential,

$$U_{\beta m, \alpha n} = \int d\mathbf{r} \left( -\frac{\partial \chi_{\beta m}^t(\mathbf{r})}{\partial E} \right) \dot{V}(\mathbf{r}, t) \chi_{\alpha n}^t(\mathbf{r}). \quad (20)$$

To prove this, we take the temporal derivative of Eq. (10), and use Eq. (8), to obtain

$$\dot{\chi}_{\alpha n}^t(\mathbf{r}) = \int d\mathbf{r}' G^t(E; \mathbf{r}, \mathbf{r}') \dot{V}(\mathbf{r}', t) \chi_{\alpha n}^t(\mathbf{r}'). \quad (21)$$

We insert this expression into Eq. (17), and carry out one of the spatial integrations using

$$\int d\mathbf{r}' G^t(E; \mathbf{r}, \mathbf{r}') \chi_{\alpha n}^t(\mathbf{r}') = -\frac{\partial \chi_{\alpha n}^t(\mathbf{r})}{\partial E}, \quad (22)$$

which follows directly by differentiating Eq. (10) with respect to the energy, and using Eq. (8) and the symmetry of the Green function  $G^t(E; \mathbf{r}, \mathbf{r}') = G^t(E; \mathbf{r}', \mathbf{r})$ . This produces the result (20).

### III. THE TWO-TERMINAL SYSTEM

Let us now confine ourselves to a nanostructure connected to two terminals, with left ( $\ell$ ) and right ( $r$ ) leads. Then we can use Eq. (16) to write the current entering the system from the left terminal in the form

$$I_\ell(t) = e \int \frac{dE}{2\pi} \sum_{nm} \left[ \left( f_\ell(E) - f_r(E) \right) \left( |S_{rm,\ell n}^t|^2 + \Re \left( S_{\ell m,\ell n}^t U_{\ell m,\ell n}^* - S_{\ell m,rn}^t U_{\ell m,rn}^* \right) \right) + \left( f_\ell(E) + f_r(E) \right) \times \Re \left( S_{\ell m,\ell n}^t U_{\ell m,\ell n}^* + S_{\ell m,rn}^t U_{\ell m,rn}^* \right) \right]. \quad (23)$$

An analogous expression holds for  $I_r(t)$ . The net current flowing in the system during a single period of the modulating potential then consists of two parts,

$$I = \oint \frac{dt}{\tau} (I_\ell(t) - I_r(t)) = I_{\text{bias}} + I_{\text{pump}}, \quad (24)$$

where the first,  $I_{\text{bias}}$ , flows only when the system is biased, whereas the second,  $I_{\text{pump}}$ , is established by the time-dependent potential (though it is affected by the chemical potential difference, when the latter is applied). Using Eqs. (19) and (20), the pumped current,  $I_{\text{pump}}$ , takes the form

$$I_{\text{pump}} = e \oint \frac{dt}{\tau} \int \frac{dE}{2\pi} \left( f_\ell(E) + f_r(E) \right) \times \frac{1}{2} \sum_m \left[ -\frac{\partial}{\partial E} \left( \langle \chi_{\ell m}^t | \dot{V} | \chi_{\ell m}^t \rangle - \langle \chi_{rm}^t | \dot{V} | \chi_{rm}^t \rangle \right) \right]. \quad (25)$$

For the biased current we find

$$I_{\text{bias}} = e \oint \frac{dt}{\tau} \int \frac{dE}{2\pi} \left( f_\ell(E) - f_r(E) \right) \times \sum_{nm} \left[ 2 |S_{rm,\ell n}^t|^2 + \Re \left( S_{\ell m,\ell n}^t U_{\ell m,\ell n}^* - S_{\ell m,rn}^t U_{\ell m,rn}^* - S_{rm,\ell n}^t U_{rm,\ell n}^* + S_{rm,rn}^t U_{rm,rn}^* \right) \right]. \quad (26)$$

The pumped part of the current,  $I_{\text{pump}}$ , can be written in terms of the temporal derivatives of the instantaneous scattering matrix. In order to vindicate this statement, we start from the asymptotic form for  $\chi_{\alpha n}^t$ , Eq. (15), for the wave going from lead  $\alpha$  into lead  $\beta$ . Noting that

$$w_{\alpha n}^-(\mathbf{r} \rightarrow \infty, \beta) = w_{\alpha n}^- \delta_{\alpha\beta} + (1 - \delta_{\alpha\beta}) \sum_m w_{\beta m}^+, \quad (27)$$

we conclude that

$$S_{\beta m,\alpha n}^t = 1 - \delta_{\alpha\beta} - i \int d\mathbf{r} \chi_{\beta m}^t(\mathbf{r}) V(\mathbf{r}, t) w_{\alpha n}^-(\mathbf{r}). \quad (28)$$

Differentiating this expression with respect to time and using Eqs. (9) and (21), yields

$$i \dot{S}_{\beta m,\alpha n}^t = \int d\mathbf{r} \chi_{\beta m}^t(\mathbf{r}) \dot{V}(\mathbf{r}, t) \chi_{\alpha n}^t(\mathbf{r}). \quad (29)$$

Note that this expression is **not** a matrix element. To turn it into an expression involving matrix elements, we use Eq. (19), by which

$$i \dot{S}_{\beta m,\alpha n}^t = \int d\mathbf{r} \dot{V}(\mathbf{r}, t) \chi_{\beta m}^t(\mathbf{r}) \times \sum_{\beta' m'} S_{\beta' m', \alpha n}^t \chi_{\beta' m'}^{t*}(\mathbf{r}). \quad (30)$$

Then, multiplying by  $S_{\beta m,\alpha n}^{t*}$  and summing over  $\alpha$  and  $n$  yields

$$\sum_{\alpha n} \dot{S}_{\beta m,\alpha n}^t S_{\beta m,\alpha n}^{t*} = -i \int d\mathbf{r} \chi_{\beta m}^{t*}(\mathbf{r}) \dot{V}(\mathbf{r}, t) \chi_{\beta m}^t(\mathbf{r}). \quad (31)$$

One notes that this identity makes the expression for  $I_{\text{pump}}$ , Eq. (25) above, to be identical with the Brouwer<sup>3</sup> formula, in the case where the system is un-biased.

In the simplest case where each of the leads is a single-channel one, the expression for the current takes a particularly simple form. In this situation, the instantaneous scattering matrix becomes a  $2 \times 2$  matrix, which can be parametrized (in the absence of a magnetic field) as

$$S^t = e^{i\psi^t} \begin{bmatrix} \sqrt{R^t} e^{i\alpha^t} & i\sqrt{T^t} \\ i\sqrt{T^t} & \sqrt{R^t} e^{-i\alpha^t} \end{bmatrix}. \quad (32)$$

Here,  $T^t$  and  $R^t$  are the instantaneous transmission and reflection, respectively. The reflection phase  $\alpha^t$  describes the asymmetry of the nanostructure. A finite time-dependent reflection phase is a necessary ingredient to obtain the pumped current. Finally,  $\psi^t$  is the transmission (Friedel) phase. With the parametrization Eq. (32) one finds, using Eqs. (29) and (31),

$$I = \frac{e}{2\pi} \oint \frac{dt}{\tau} \int dE \left[ \left( f_\ell(E) - f_r(E) \right) \left[ 2T^t - \frac{1}{2} \left( \frac{\partial}{\partial E} \left( (R^t - T^t) \frac{d\psi^t}{dt} \right) + \frac{d}{dt} \left( (R^t - T^t) \frac{\partial \psi^t}{\partial E} \right) \right) \right] + \left( f_\ell(E) + f_r(E) \right) \frac{\partial}{\partial E} \left( R^t \frac{d\alpha^t}{dt} \right) \right]. \quad (33)$$

The charge passing through the nanostructure during a single period of the potential,  $Q$ , is then

$$Q = Q_{\text{bias}} + Q_{\text{pump}}. \quad (34)$$

Here,

$$Q_{\text{bias}} = \frac{e}{2\pi} \oint dt \int dE \left[ (f_\ell(E) - f_r(E)) 2T^t + \frac{\partial}{\partial E} (f_\ell(E) - f_r(E)) T^t \frac{d\psi^t}{dt} \right]. \quad (35)$$

It is seen that the first term here is just the Landauer formula, with the transmission coefficient averaged over the temporal period. The second term forms a correction to this result, brought about by the modulating potential. The pumped charge is given by

$$Q_{\text{pump}} = -\frac{e}{2\pi} \oint dt \int dE \times \frac{\partial}{\partial E} (f_\ell(E) + f_r(E)) R^t \frac{d\alpha^t}{dt}, \quad (36)$$

(see Ref. 6), and it vanishes unless  $\alpha^t$  is time-dependent.

### A. Example—the single-level quantum dot

Clearly, a comparison between  $Q_{\text{pump}}$  and the second part of  $Q_{\text{bias}}$  is called for. Consider for simplicity zero temperature. Then,  $Q_{\text{pump}}$  is given by the values of  $R^t d\alpha^t/dt$  at  $E = E_F \pm \delta\mu/e$ , where  $\delta\mu$  is the chemical potential difference, and  $E_F$  denotes the Fermi level. On the other hand, the second term in  $Q_{\text{bias}}$  is given by  $\sim \int dE [-(\delta\mu/e)(\partial^2 f/\partial E^2) T^t (d\psi^t/dt)]$ , and hence should be much smaller than the Landauer contribution, which is proportional to  $\delta\mu/e$ . Nevertheless, it may be of interest to explore this term experimentally, as it is related to the Friedel phase of the nanostructure.

To further explore this point, we consider the following simple example: a quantum dot, with a single localized level, coupled to two ideal 1D leads.<sup>25</sup> Adopting the tight-binding description, we model the two leads connecting the quantum dot to the electronic reservoirs by 1D chains of sites, whose on-site energies are assumed to vanish, and whose nearest-neighbor transfer amplitudes are denoted by  $-J$ . Thus the energy of an electron of wave vector  $k$  moving on such a chain is

$$E_k = -2J \cos ka, \quad (37)$$

where  $a$  is the lattice constant. The localized level, of energy  $\epsilon_0$ , is attached to the left-hand-side lead with matrix element  $-J_\ell$ , and to the right-hand-side lead with matrix element  $-J_r$ . The latter two quantities are assumed to vary slowly in time, in a periodic way. Our formalism requires just the knowledge of the instantaneous scattering matrix of the system. For the case at hand,

$$S^t = \begin{bmatrix} -1 + \left(\frac{J_\ell}{J}\right)^2 M_k & \frac{J_\ell J_r}{J} M_k \\ \frac{J_\ell J_r}{J} M_k & -1 + \left(\frac{J_r}{J}\right)^2 M_k \end{bmatrix}, \quad (38)$$

with

$$M_k = \frac{2iJ \sin ka}{E_k - \epsilon_0 + e^{ika}(J_\ell^2 + J_r^2)/J}. \quad (39)$$

Let us consider first the pumped charge. At zero temperature, it is given by

$$Q_{\text{pump}} = \frac{e}{2\pi} \oint dt R^t \frac{d\alpha^t}{dt} = \frac{e}{2\pi} \oint dt \frac{\sin ka}{|E_k - \epsilon_0 + e^{ika}(X_\ell + X_r)|^2} \times [(\dot{X}_\ell - \dot{X}_r)(\epsilon_0 - E_k) + E_k(X_r \dot{X}_\ell - X_\ell \dot{X}_r)], \quad (40)$$

in which energies are measure in units of  $J$ , and

$$X_\ell \equiv \left(\frac{J_\ell}{J}\right)^2, \quad X_r \equiv \left(\frac{J_r}{J}\right)^2, \quad (41)$$

are the time-dependent parameters of the system. Note that these two parameters can be thought of as the ‘contact conductances’ of the quantum dot. Now imagine those to vary in time as follows: Initially, both are equal to  $X_1$ . Then  $X_\ell$  is increased linearly in time until it reaches the value  $X_2$ , while  $X_r$  is being held fixed at the value  $X_1$ . From that point,  $X_\ell$  is held fixed, while  $X_r$  increases linearly to the value  $X_2$ , and so on, see Fig. 1.

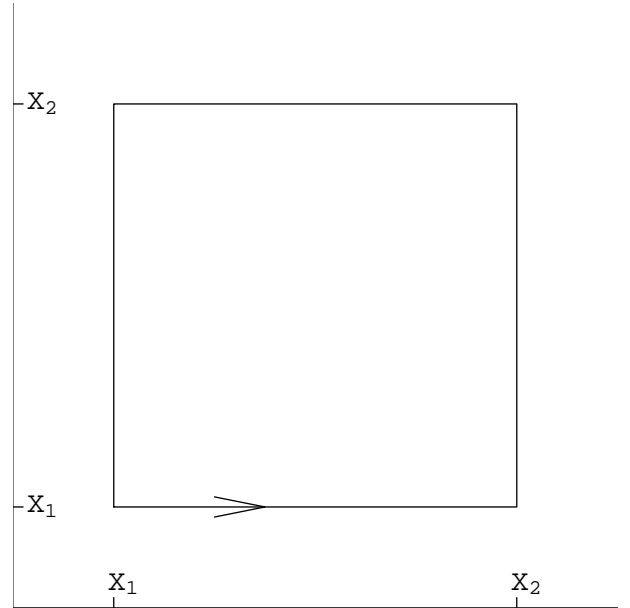


FIG. 1. The periodic temporal evolution of the parameters  $X_\ell$  and  $X_r$  in the parameter plane.

It is quite straightforward to find  $Q_{\text{pump}}$  for such a cycle. One obtains

$$Q_{\text{pump}} = \frac{e}{\pi} \int_{X_1}^{X_2} dX \left( F(X; X_1) - F(X; X_2) \right), \quad (42)$$

with

$$F(X; Z) = \frac{\sin ka(\epsilon_0 - E_k + E_k Z)}{|E_k - \epsilon_0 + e^{ika}(X + Z)|^2}. \quad (43)$$

The resulting charge differs significantly from zero, and approaches unity (in units of  $e$ ) as long as the line of maximal transmission in the  $X_\ell$ - $X_r$ -plane is well within the closed orbit forming the period.<sup>9</sup> In the present model, that line is given by

$$X_\ell + X_r = 2 \frac{E_k - \epsilon_0}{E_k}. \quad (44)$$

We will elaborate on this point, which is exemplified in Fig. 2, in a future publication. For the parameters used to produce the results shown in Fig. 2, for  $X_1 = 0$  the maximal transmission line is contained within the pumping contour (see Fig. 1), while for its higher values the pumping contour shifts away from the maximal transmission line.

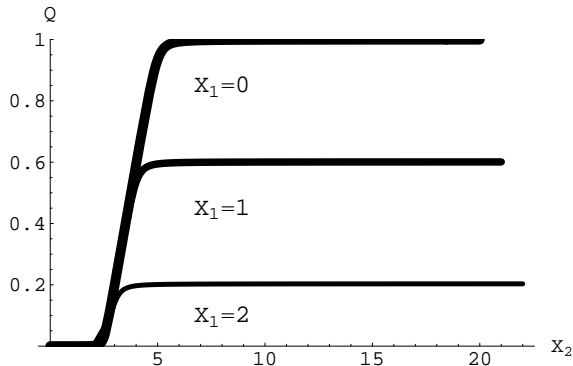


FIG. 2. The pumped charge (in units of  $e$ ) as function of  $X_2$ , for several values of  $X_1$ , indicated on the figure. Here  $ka = \pi - 0.1$ , and  $\epsilon_0 = -3$ .

Let us next consider the time-average that appears in the second term of the biased current, i.e.,  $\oint T^t d\psi^t / dt$ . In our example, this quantity becomes

$$\oint dt T^t \frac{d\psi^t}{dt} = - \oint dt \frac{4 \sin^3 ka (E_k - \epsilon_0) X_\ell X_r (\dot{X}_\ell + \dot{X}_r)}{|E_k - \epsilon_0 + e^{ika}(X_\ell + X_r)|^4}. \quad (45)$$

On a symmetric periodical curve like that presented in Fig. 1 this integral vanishes. Hence, in such a symmetric

configuration, there will be no deviation from the Landauer formula due to the temporal variation of the Friedel phase. One may conclude from this example that when the pumping orbit in the plane of the time-dependent parameters is not so simple as the one considered above, there might be a small correction, related to the asymmetry of the orbit.

#### IV. CONCLUDING REMARKS

The motivation of this work is mainly to examine the validity of the adiabatic approximation in calculating the charge pumped quantum-mechanically through a confined system of non-interacting electrons, and to study the effects of a constant bias. To this end, we have derived the time-dependent current generated when the system is subject to a slowly-changing modulating potential, in addition to being connected to reservoirs of different chemical potentials. We have found that the widely-used Brouwer formula which gives the pumped charge in terms of the instantaneous scattering matrix is valid for arbitrary amplitudes of the modulating potential, as long as the lowest-order adiabatic approximation can be employed.

In the process, we have obtained an alternative expression for the pumped charge, Eq. (1), which gives it in terms of matrix elements of the temporal derivative of the potential between the instantaneous scattering states. We have also derived and analyzed the effects of the modulating potential on the biased current, and showed them to be quite small. Our formalism allows for the possibility to obtain systematically the corrections to the lowest-order adiabatic approximation.

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#### APPENDIX A: CORRECTIONS TO THE ADIABATIC APPROXIMATION

The results presented above have been obtained in the adiabatic approximation, in which only first derivatives with respect to time are kept. As stated above, this means that in the iterative solution of Eq. (7) only the first iteration has been maintained. Here we discuss the

contribution of the next iteration. For the sake of simplicity, we carry out this calculation for an un-biased system with two single-channel leads.

To second order in the temporal derivative, the scattering solution can be presented in the form

$$\chi(\mathbf{r}, t) = \chi^t(\mathbf{r}) - i \int d\mathbf{r}' G^t(E; \mathbf{r}, \mathbf{r}') \left( \dot{\chi}_\alpha^t(\mathbf{r}') + \Delta \dot{\chi}_\alpha^t(\mathbf{r}') \right), \quad (\text{A1})$$

with

$$\Delta \dot{\chi}_\alpha^t(\mathbf{r}') = -i \int d\mathbf{r}'' \frac{d}{dt} \left( G^t(E; \mathbf{r}', \mathbf{r}'') \dot{\chi}_\alpha^t(\mathbf{r}'') \right). \quad (\text{A2})$$

It follows that the quantity  $U$ , Eq. (17), is now modified into

$$\begin{aligned} \tilde{U}_{\beta\alpha} &= U_{\beta\alpha} + \Delta U_{\beta\alpha}, \\ U_{\beta\alpha} &= \int d\mathbf{r} \chi_\beta^t(\mathbf{r}) \dot{\chi}_\alpha^t(\mathbf{r}), \\ \Delta U_{\beta\alpha} &= \int d\mathbf{r} \chi_\beta^t(\mathbf{r}) \Delta \dot{\chi}_\alpha^t(\mathbf{r}). \end{aligned} \quad (\text{A3})$$

As a result, we find that the current entering lead  $\beta$  consists of two parts, the leading order in the adiabatic approximation,  $I_\beta$ , which has been discussed above, and a correction,  $\Delta I_\beta$ . Explicitly,

$$\begin{aligned} \tilde{I}_\beta(t) &= I_\beta(t) + \Delta I_\beta(t), \\ I_\beta(t) &= e \int \frac{dE}{2\pi} \sum_\alpha f_\alpha(E) \\ &\quad \times \left[ \delta_{\alpha\beta} - |S_{\beta\alpha}^t|^2 + 2\Re(S_{\beta\alpha}^{t*} U_{\beta\alpha}) \right], \\ \Delta I_\beta(t) &= e \int \frac{dE}{2\pi} \sum_\alpha f_\alpha(E) \\ &\quad \times \left[ -|U_{\beta\alpha}|^2 + 2\Re(S_{\beta\alpha}^{t*} \Delta U_{\beta\alpha}) \right]. \end{aligned} \quad (\text{A4})$$

Let us first verify that the correction  $\Delta I_\beta$  obeys charge conservation over the entire period. To this end, we sum  $\Delta I_\beta$  over  $\beta$ . Using Eq. (19), we have

$$\begin{aligned} &\sum_\beta \left[ |U_{\beta\alpha}|^2 - 2\Re(S_{\beta\alpha}^{t*} \Delta U_{\beta\alpha}) \right] \\ &= \int d\mathbf{r} \int d\mathbf{r}' \left[ \sum_\beta \chi_\beta^t(\mathbf{r}) \dot{\chi}_\alpha^t(\mathbf{r}) \chi_\beta^{t*}(\mathbf{r}') \dot{\chi}_\alpha^{t*}(\mathbf{r}') \right. \\ &\quad \left. - 2\Im \left( \chi_\alpha^{t*}(\mathbf{r}) \frac{d}{dt} G^t(E; \mathbf{r}, \mathbf{r}') \dot{\chi}_\alpha^t(\mathbf{r}') \right) \right]. \end{aligned} \quad (\text{A5})$$

We can now employ the fact that the current should be conserved upon integrating over the entire period, that is, when expression (A5) is inserted into  $\oint dt$ . Then we may integrate the second term by parts. Consequently, using the relation<sup>22</sup>

$$\sum_\alpha \chi_\alpha^t(\mathbf{r}) \chi_\alpha^{t*}(\mathbf{r}') = -2\Im G^t(E; \mathbf{r}, \mathbf{r}'), \quad (\text{A6})$$

the two terms in (A5) exactly cancel one another.

Let us now turn to the expression for the correction  $\Delta I_\beta$ , Eq. (A4), and insert there the condition that the system is un-biased, i.e.,  $f_\alpha(E) = f(E)$ . Then, using Eqs. (19), (21), (22), and (A6), we find

$$\begin{aligned} \sum_\alpha |U_{\beta\alpha}|^2 &= -2 \int d\mathbf{r} \int d\mathbf{r}' \left( \frac{\partial \chi_\beta^t(\mathbf{r})}{\partial E} \right) \dot{V}(\mathbf{r}, t) \\ &\quad \times \Im \left( G^t(E; \mathbf{r}, \mathbf{r}') \right) \dot{V}(\mathbf{r}', t) \left( \frac{\partial \chi_\beta^{t*}(\mathbf{r}')}{\partial E} \right), \end{aligned} \quad (\text{A7})$$

and

$$\begin{aligned} 2\Re \sum_\alpha S_{\beta\alpha}^{t*} \Delta U_{\beta\alpha} &= 2\Im \int d\mathbf{r} \int d\mathbf{r}' \left[ \left( \frac{\partial \chi_\beta^t(\mathbf{r})}{\partial E} \right) \dot{V}(\mathbf{r}, t) \right. \\ &\quad \times \left( \frac{\partial G^t(E; \mathbf{r}, \mathbf{r}')}{\partial E} \right) \dot{V}(\mathbf{r}', t) \chi_\beta^{t*}(\mathbf{r}') \\ &\quad + \left( \frac{\partial^2 \chi_\beta^t(\mathbf{r})}{\partial E^2} \right) \dot{V}(\mathbf{r}, t) G^t(E; \mathbf{r}, \mathbf{r}') \dot{V}(\mathbf{r}', t) \chi_\beta^{t*}(\mathbf{r}') \Big] \\ &\quad + \Im \int d\mathbf{r} \left( \frac{\partial^2 \chi_\beta^t(\mathbf{r})}{\partial E^2} \right) \ddot{V}(\mathbf{r}, t) \chi_\beta^{t*}(\mathbf{r}). \end{aligned} \quad (\text{A8})$$

To obtain the last equality, we have made use of the relations

$$\frac{\partial^2 \chi_\beta^t(\mathbf{r})}{\partial E^2} = -2 \int d\mathbf{r}' \left( \frac{\partial \chi_\beta^t(\mathbf{r}')}{\partial E} \right) G^t(E; \mathbf{r}', \mathbf{r}), \quad (\text{A9})$$

and

$$\begin{aligned} &\dot{G}^t(E; \mathbf{r}, \mathbf{r}') \\ &= \int d\mathbf{r}_1 G^t(E; \mathbf{r}, \mathbf{r}_1) \dot{V}(\mathbf{r}_1, t) G^t(E; \mathbf{r}_1, \mathbf{r}'). \end{aligned} \quad (\text{A10})$$

Both relations are obtained by taking derivatives of Eqs. (8) and (10) with respect to the energy and the time.

Collecting all these terms, we obtain

$$\begin{aligned} \Delta I_\beta(t) &= \frac{-e}{\pi} \int dE f(E) \\ &\quad \times \Im \frac{\partial}{\partial E} \langle \chi_\beta^t | \dot{V}(t) \dot{G}^t(E) + \frac{1}{2} \ddot{V}(t) G^t(E) | \chi_\beta^t \rangle. \end{aligned} \quad (\text{A11})$$

It is satisfactory to note that, again, (upon integrating by parts with respect to the energy), the energy integral includes the derivative of the Fermi function. Hence, up to the second-order in the adiabatic approximation, we find

$$\begin{aligned} \tilde{I}_\beta(t) &= \frac{e}{2\pi} \int dE \left( \frac{\partial f(E)}{\partial E} \right) \left[ \langle \chi_\beta^t | \dot{V} | \chi_\beta^t \rangle \right. \\ &\quad \left. + \Im \left( \langle \chi_\beta^t | 2\dot{V}(t) \dot{G}^t(E) + \ddot{V}(t) G^t(E) | \chi_\beta^t \rangle \right) \right]. \end{aligned} \quad (\text{A12})$$

To estimate the relative magnitude of the correction (the second term above) compared to the leading order one (the first term there), consider the part including the

second derivative of the potential. Using Eq. (22), this part becomes

$$\int d\mathbf{r} \chi_{\beta}^{t*}(\mathbf{r}) \ddot{V}(\mathbf{r}, t) \left( -\frac{\partial \chi_{\beta}^t(\mathbf{r})}{\partial E} \right). \quad (\text{A13})$$

It follows that the correction will be smaller than the leading order term by a factor proportional to  $1/\tau$ , due to the extra temporal derivative, times the energy derivative of the instantaneous scattering state. The latter will include the energy-derivatives of the instantaneous transmission and reflection amplitudes (which appear in  $\chi^t$ ), and possibly a term proportional to the 1D density of states, i.e., the velocity, (coming, e.g., from the factors  $e^{ika}$  which appear in  $\chi^t$  of our simple example discussed in Sec. III). We may conclude that as long as the energy derivative of the instantaneous scattering solution is small on the scale of  $\omega \propto 1/\tau$ , the leading order adiabatic approximation suffices to obtain the pumped charge.

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<sup>1</sup> B. L. Altshuler and L. I. Glazman, *Science* **283**, 1864 (1999).

<sup>2</sup> F. Hekking and Yu. V. Nazarov, *Phys. Rev. B* **44**, 9110 (1991).

<sup>3</sup> P. W. Brouwer, *Phys. Rev. B* **58**, R10135 (1998).

<sup>4</sup> I. L. Aleiner and A. V. Andreev, *Phys. Rev. Lett.* **81**, 1286 (1998).

<sup>5</sup> F. Zhou, B. Spivak, and B. L. Altshuler, *Phys. Rev. Lett.* **82**, 608 (1999).

<sup>6</sup> T. A. Shutenko, I. L. Aleiner and B. L. Altshuler, *Phys. Rev. B* **61**, 10366 (2000).

<sup>7</sup> S. H. Simon, *Phys. Rev. B* **61**, R16327 (2000).

<sup>8</sup> P. A. Maksym, *Phys. Rev. B* **61**, 4727 (2000).

<sup>9</sup> Y. Levinson, O. Entin-Wohlman, and P. Wölfle, *cond-mat/0010494* (2000).

<sup>10</sup> Y. Wei, J. Wang, and H. Gou, *Phys. Rev. B* **62**, 9947 (2000).

<sup>11</sup> M. Moskalets and M. Büttiker, *cond-mat/0108061* (2001).

<sup>12</sup> P. Sharma and C. Chamon, *Phys. Rev. Lett.* **87**, 096401 (2001).

<sup>13</sup> Y. Makhlin and A. Mirlin, *Phys. Rev. Lett.* **87**, 276803 (2001).

<sup>14</sup> Y. Wei, J. Wang, H. Guo, and C. Roland, *Phys. Rev. B* **64**, 115321 (2001).

<sup>15</sup> M. Switkes, C. M. Marcus, K. Campman and A. C. Gosard, *Science* **283**, 1905 (1999).

<sup>16</sup> H. Pothier, P. Lafarge, U. Urbina, D. Esteve and M. H. Devoret, *Europhys. Lett.* **17**, 249 (1992).

<sup>17</sup> L. P. Kouwenhoven, A. T. Johnson, N. C. van der Vaart, A. van der Enden, C. J. P. M. Harmans, and C. T. Foxon, *Z. Phys.* **B85**, 381 (1991).

<sup>18</sup> D. J. Thouless, *Phys. Rev. B* **27**, 6083 (1983).

<sup>19</sup> M. Büttiker, H. Thomas, and A. Prêtre, *Z. Phys.* **B94**, 133 (1994).

<sup>20</sup> J. E. Avron, A. Elgart, G. M. Graf, and L. Sadun, *Phys. Rev. B* **62**, R10 618 (2000).

<sup>21</sup> A. Aharony and O. Entin-Wohlman, *cond-mat/0111053* (2001).

<sup>22</sup> Y. Levinson, *Phys. Rev. B* **61**, 4748 (2000).

<sup>23</sup> O. Entin-Wohlman, Y. Levinson, and P. Wölfle, *Phys. Rev. B* **64**, 195308 (2001).

<sup>24</sup> Y. Levinson and P. Wölfle, *Phys. Rev. Lett.* **83**, 1399 (1999).

<sup>25</sup> T. K. Ng and P. A. Lee, *Phys. Rev. Lett.* **61**, 1768 (1988).